

Chlorthal-dimethyl
1861-32-1 | DTXSID0024000

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 8.97

Global applicability domain: Inside

Local applicability domain index: 9.67e-01

Confidence level: 8.36e-01

Nearest Neighbors from the Training Set

| | | |
|---|--|---|
| <div>Image not found</div> <div>2,3,7-Trichlorodibenzo-p-dioxin</div> <div>Measured: 9.14</div> <div>Predicted: 8.95</div> | <div>Image not found</div> <div>1,2,4-Trichlorodibenzo-1,4-dioxin</div> <div>Measured: 8.97</div> <div>Predicted: 8.77</div> | <div>Image not found</div> <div>1,2,3,5,7-Pentachloronaphthalene</div> <div>Measured: 8.82</div> <div>Predicted: 8.95</div> |
| <div>Image not found</div> <div>1,2,3,5,8-Pentachloronaphthalene</div> <div>Measured: 9.10</div> <div>Predicted: 8.95</div> | <div>Image not found</div> <div>Pyrene</div> <div>Measured: 8.80</div> <div>Predicted: 8.87</div> | |